Evaluation and Improvement of Molecular Simulation Methods

NIST researchers are facilitating the use of molecular simulation methods by the leading the effort to fill two major obstacles to its implementation provide molecular interaction models and data simulation code.

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Molecular simulation has been identified as a "breakthrough technology" for the estimation of fluid properties of industrial importance. It would improve the productivity of data generation and enhance the computational capabilities of industrial researchers. There are obstacles to realizing the breakthrough. The obstacles are the lack of molecular interaction models that contain the necessary physics for the molecules of interest and the availability of simulation codes that can adequately sample the fluid system in an acceptable time frame. The interest in molecular simulation is to determine fluid thermal properties for systems/conditions where data are lacking and direct measurement would be expensive and/or hazardous such as highly flammable materials or high temperature, high pressure states.

NIST is addressing the obstacles in two distinct ways. The development of improved interaction models for industrially interesting fluids is being encouraged through leadership in the activities of the ***Industrial Fluid Properties Simulation Collective (IFPSC)***, an association of industrial and government scientists interested developing and applying molecular simulation to industrially significant fluid property determination problems. The operation of the series of Industrial Fluid Property Simulation Challenges is the major activity of the IFPSC. The results of the first two challenges have identified situations where simulation methods can be improved to make them more robust and computationally efficient. These are the determination of fluid-fluid phase boundaries and the determination of the shear viscosity and thermal conductivity transport coefficients. NIST is actively involved in both problems and have found and evaluated simulation methods that satisfy the robust and efficient conditions.

Researchers from NIST and the University of New York have extended the Grand Canonical Ensemble Transfer Matrix Monte Carlo method to enable a simulation to determine liquid-vapor and liquid-liquid phase boundaries for mixtures with greater computational efficiency than existing methods.

The relevant codes are being incorporated into a public access Monte Carlo package, "Towhee", that is currently maintained by Sandia National Laboratory. This method has also been applied to simple models of protein denaturation.

The estimation of transport coefficients through molecular simulation tends to be a computationally intensive business because of the large amount of sampling required to obtain converged results. The reversed-perturbation molecular dynamics method has been evaluated and shown to be computationally more efficient than the other available methods for estimating the shear viscosity and thermal conductivity of liquids as shorter computation times are needed for convergence. It is not useful for gases as very large systems are necessary to have it work for gases.

Publications:

1. J. R. Errington and V. K. Shen, J. Chem. Phys. **123**, 164103 (2005)
2. V. K. Shen, *et al*, J. Biophysical Journal **90**, 1949 (2006)
3. R. D. Mountain, J. Chem. Phys. **124**, 104109 (2006)